Equation (#) on the problem sheet will be referred to as equation (s#).

Problem 1

(a)

$$H = \frac{p^2}{2m} + V(q), \quad \frac{\partial H}{\partial q} = \partial_q V(q) = -\dot{p}, \quad \frac{\partial H}{\partial p} = \frac{p}{m} = \dot{q}$$

(b) We calculate $\partial_q V(q)$ explicitly and using the result of (a) we find

$$\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \begin{pmatrix} q - q^3 \\ p/m \end{pmatrix}.$$

Note that ϕ does not explicitly depend on time! In order to solve these differential equations uniquely we need two initial values, since they reduce to an uncoupled differential equation of second order:

$$m\ddot{q} = q - q^3,$$

where p is obtained by calculating $m\mathrm{d}_t q$.

(c) We rewrite equation (s4):

$$\dot{p} = \mu(1 - q^2)p - q - \Theta(\lambda),$$

which is already our first line of the equation. The rest follows simply by definition:

$$\dot{q} = p, \quad \dot{\lambda} = 1,$$

which yields

$$\begin{pmatrix} \dot{p} \\ \dot{q} \\ \dot{\lambda} \end{pmatrix} = \begin{pmatrix} \mu(1 - q^2)p - q - \Theta(\lambda) \\ p \\ 1 \end{pmatrix}. \tag{1}$$

Since g_2 is identified with x, a vector $\mathbf{g}$ that solves eq.(1), provides an x that solves eq.(s4).

(d) The ODE of a harmonic oscillator in the above notation would be

$$\begin{pmatrix} \dot{p} \\ \dot{q} \\ \dot{\lambda} \end{pmatrix} = \begin{pmatrix} -\omega^2 q \\ p \\ 1 \end{pmatrix}.$$

Since the problem is time-translationary invariant, the free parameter in the bottom line is irrelevant for the physics. Solving the middle line yields one free parameter q_0:

$$q(t) - q_0 = \int_0^t \mathrm{d}t' p(t').$$

Plugging this into the first line, and solving for p we obtain another free parameter. For N_A particles we obtain one ODE of second order for each particle and each spatial dimension. Thus for a unique solution, we need $6N_A$ initial conditions.

(e) We rearrange equation (s5):

$$\frac{r_k - r_{k-1}}{\Delta t} = f(r_{k-1}, (k-1)/N),$$

where the limit $\Delta t \longrightarrow 0$ on the left-hand side yields the definition of the time derivative of $r(t)$. Furthermore on the right-hand side $(k-1)/N \longrightarrow t = const.$ since both k and N grow in the same fashion.

(f) We first choose the potential

$$V_1(q) = \frac{1}{2}q^2\left(\frac{1}{2}q^2 - 1\right) + \frac{1}{20}\cos(40q)$$

which is depicted in the LHS of figure 1. The RHS contains a prediction for the behaviour of different particles given a square centered around (0,0) in phase space as the set of initial points.

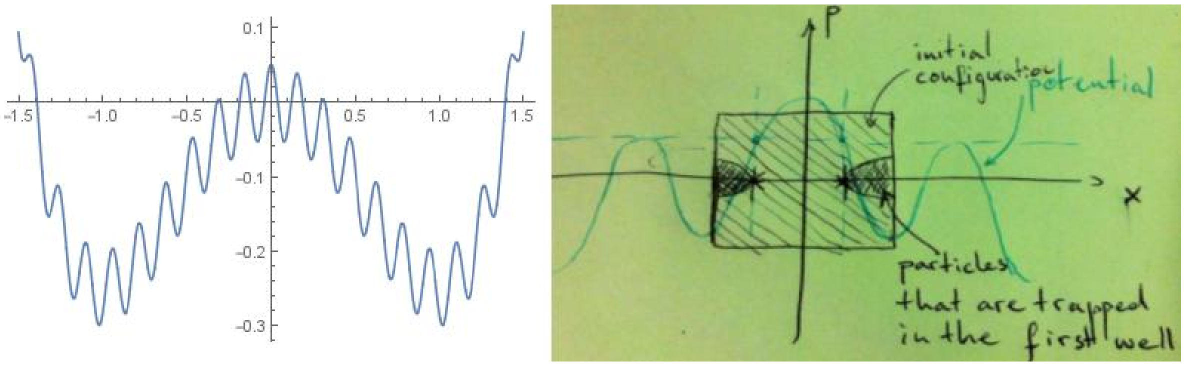

Figure 1: Left-hand side: Plot of the potential $V_1(q)$. Right-hand side: The square represents the set of particles in their initial phase space configuration. Note that the black stars on the x-axis represent particles with zero momentum and initial potential energy of the summit of the neighboring 'hill', as seen by the green horizontal line. Particles outwards from these points will certainly be trapped. But also some particles furtherout with non-zero initial momentum, as indicated by the darkly shaded areas. If the initial momentum is high enough though, the particles will escape the first well nonetheless.

The predicted behaviour can be seen in the animation **V1.gif** of the time evolution of phase space. The great loop clearly reflects the mexican-hat-potential in $V_1(q)$.

Subsequently we evaluated the phase space dynamics for the potential

$$V_2(x) = 0.1 \cdot \left[(x-1)^2 + \frac{1}{1.8 + 10^5(x-0.5)^2} + \frac{1}{1.1 + 10^5(x-0.9)^2}\right],$$

which is depicted in figure 2.

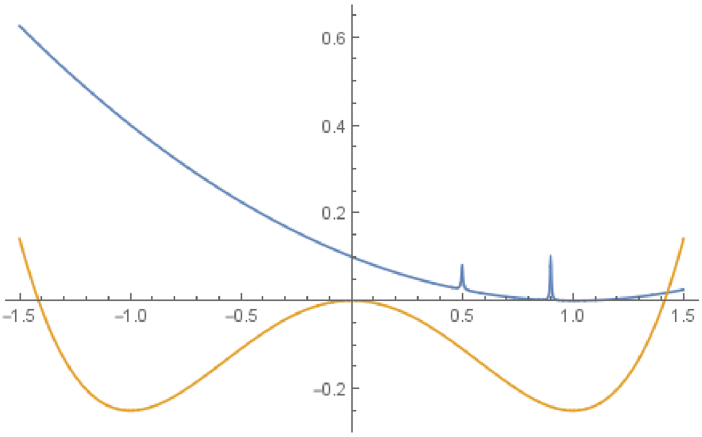

Figure 2: Plot of the potential V_2 (blue line) and the mexican hat potential (yellow line), which has an overall harmonic shape but exhibits to narrow scatterers which reflect some particles and hence lead to three different cycling frequencies, which we describe by the name 'phase space race'.

The dynamics can be seen in **V2.gif** and clearly exhibit the movement of three different bulks in phase space.

Finally we created a rather 'random' potential

$$V_3(x) = 0.1 \cdot \left[\sin(20x) + \cos(15x^2 + 1) + \frac{1}{2 + 10^4(x + 1.5)^2} + \frac{1}{1.5 + 10^4(x - 1.5)^2} \right],$$

where the last two terms are peaks to keep particles from escaping a finite domain.

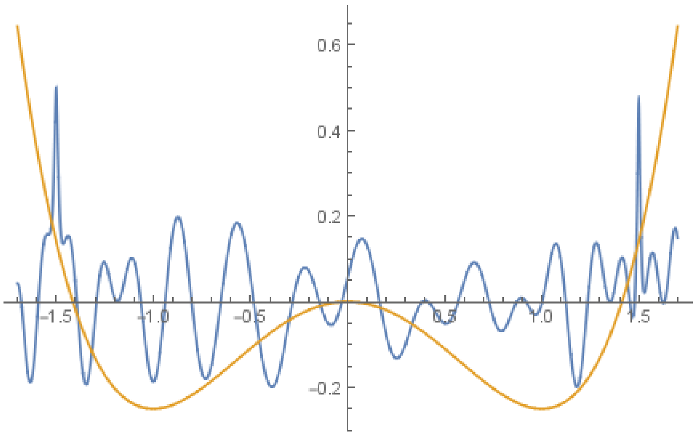

Figure 3: Plot of the potential V_3 (blue line) and the mexican hat potential (yellow line).

The dynamics can be seen in **V3.gif**, where some particles in the left part of the initial region are trapped, by the same mechanism as in V_1. It is clear to see, that a connection of the upper and the lower particle stream in phase space (this happens when particles get scattered back) can only happen when the particles encounter a peak of greater hight than ever before on their way out.

Shearing into a rhombus: This behaviour should be expected for all well-behaved potentials in a sufficiently small time intervall starting from the $t = 0$. Since the particles in the upper (lower) part of the square have momentum towards the right (left), they will, in the first instant of time evolution, simply move towards the right (left) with a speed according to their distance to the x-axis.

(h) Yes!